SIMULATION OF FLOW AND PARTICLE TRANSPORT AND DEPOSITION IN POROUS MEDIA WITH COMPUTATIONAL FLUID DYNAMICS

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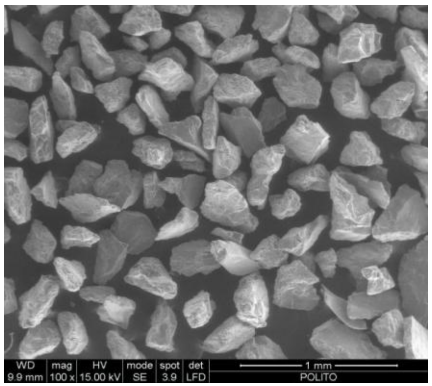

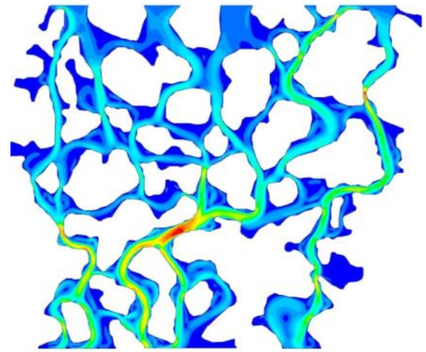

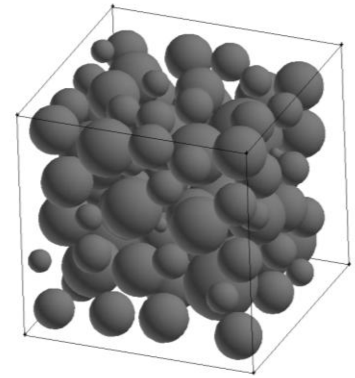

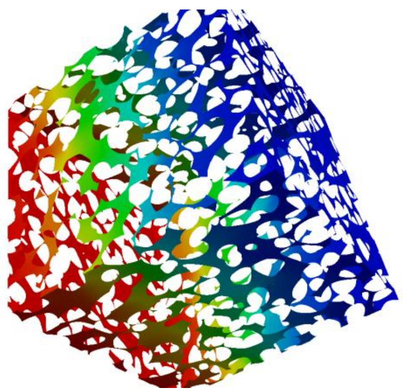

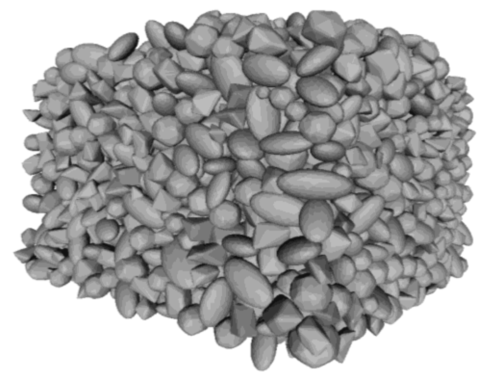

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ECCE9/ECAB2

The Hague, Netherlands

Introduction: motivation of the work

Many fields of interest:

- Process Engg.: Packed bed reactors
  Filtration
  Chromatographic separation
- Environmental Engg.: Aquifer remediation

Purpose

Results from microscale simulations … → … used to develop macroscale models

".. since, depending on the right scale of observation, everything is porous. "

Theoretical background: fluid flow

Macroscale Pseudo-Continuum Approach

- Creeping flow (Re < 1): linear relationship

Darcy's law
$$\frac{\Delta P}{L} = \frac{\mu}{k}\, q$$

- Re > 1: nonlinear relationship

Forchheimer's law
$$\frac{\Delta P}{L} = \frac{\mu}{k}\, q + \beta\, \rho\, q^2$$

- Packed beds filter law (wide range of Re)

$$\Delta P^* = \frac{\Delta P \rho D_g \varepsilon^3}{L G_0^2 (1-\varepsilon^3)}$$

Ergun's law
$$\Delta P^* = \frac{150}{Re^*} + 1.75$$

$$Re^* = \frac{D_g G_0}{(1-\varepsilon)\mu}$$

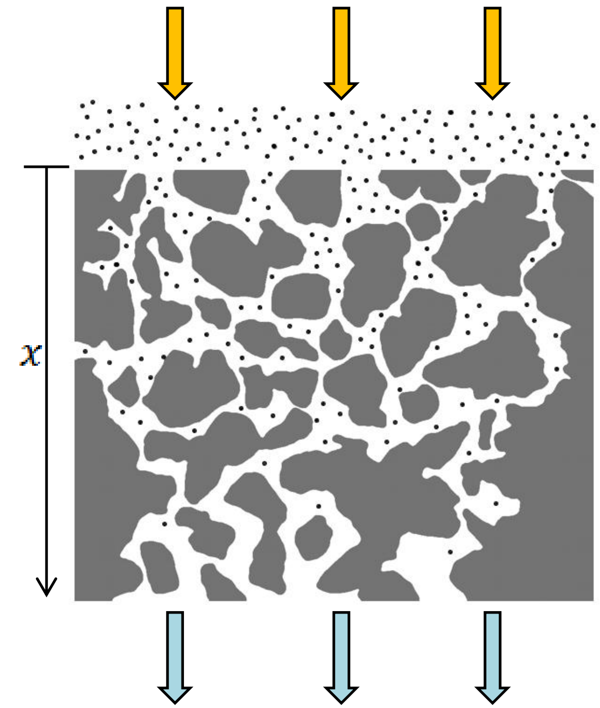
THEORETICAL BACKGROUND: PARTICLE DEPOSITION

MACROSCALE 1D ADVECTIVE-DIFFUSIVE EQUATION

$$\frac{\partial C}{\partial t} + q\frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial x^2} = Source$$

$$Source = -K_d C$$

$$K_d = \frac{3}{2}\frac{1-\varepsilon}{\varepsilon}\frac{q}{D_g}\alpha\,\eta$$



η : <u>COLLECTOR DEPOSITION EFFICIENCY</u>

THEORETICAL BACKGROUND: PARTICLE DEPOSITION

DEPOSITION EFFICIENCY

- BROWNIAN DIFFUSION

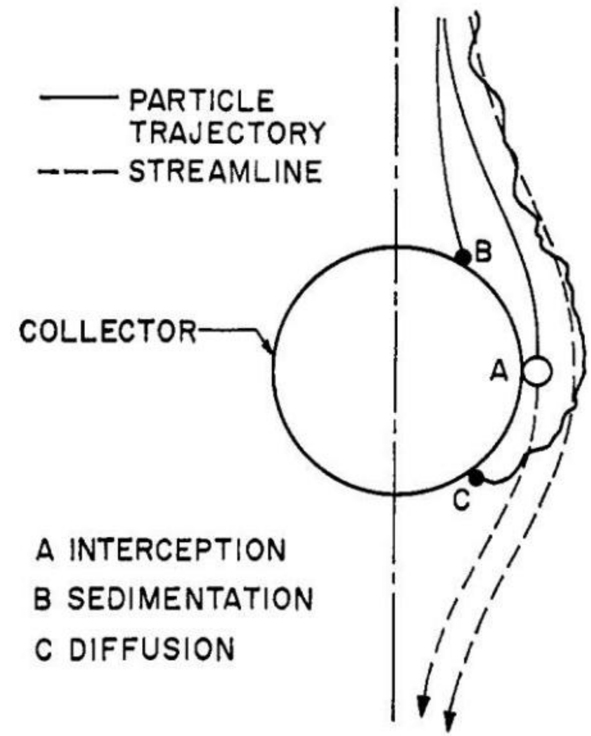
$$\eta_B = 4.04 Pe^{-\frac{2}{3}}$$ LEVICH

$$\eta_B = 4\, As^{\frac{1}{3}}\, Pe^{-\frac{2}{3}}$$ HAPPEL

- INTERCEPTION

$$\eta_I = \frac{3}{2}\left(\frac{d_p}{D_g}\right)^2 = \frac{3}{2}\, N_R^2$$ YAO

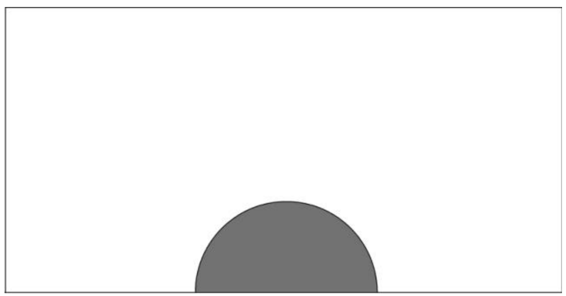
$$\eta_I = \frac{3}{2}\, As\, N_R^2$$ HAPPEL



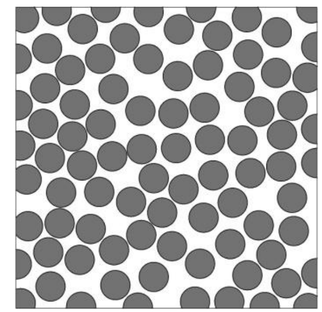
METHODOLOGY: MICROSCALE GEOMETRIC MODELS

INCREASING COMPLEXITY

– SINGLE COLLECTOR
– CIRCULAR SHAPE
(under axial simmetry)

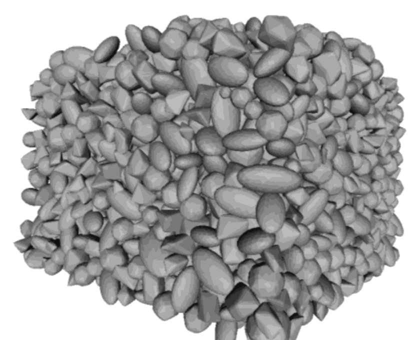


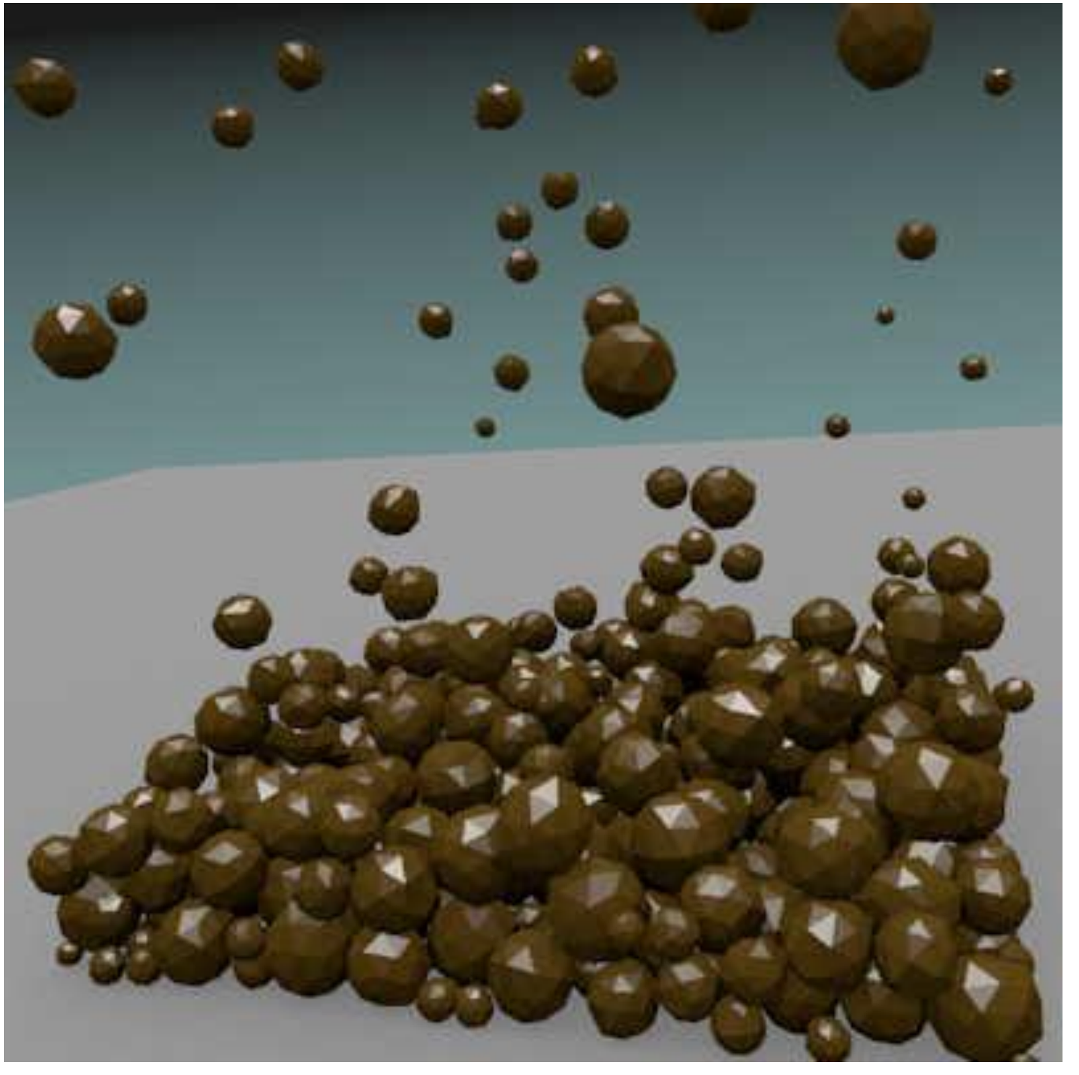
– CIRCULAR SHAPE
– ARTIFICIAL PACKING
(planar geometry)



– IRREGULAR SHAPES
– REALISTIC μ-CT/SEM SCANS
(planar geometry)

– IRREGULAR SHAPES
– ARTIFICIAL PACKING





Methodology: operating conditions

Solvers and Meshing

- Finite volume CFD codes:

FLUENT, OPENFOAM

- Body-fitted meshers:

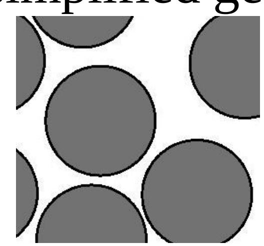
GAMBIT, SNAPPYHEXMESH

Operating Conditions

- D_g = 100 m ÷ 300 m
- = 0,3 ÷ 0,5
- $q = 10^{-6}, 10^{-5}, \ldots, 10^{-1}$ m s^{-1}
- Laminar model
- T = 293 K
- Viscosity = 0.00103 Kg m^{-1}s^{-1}

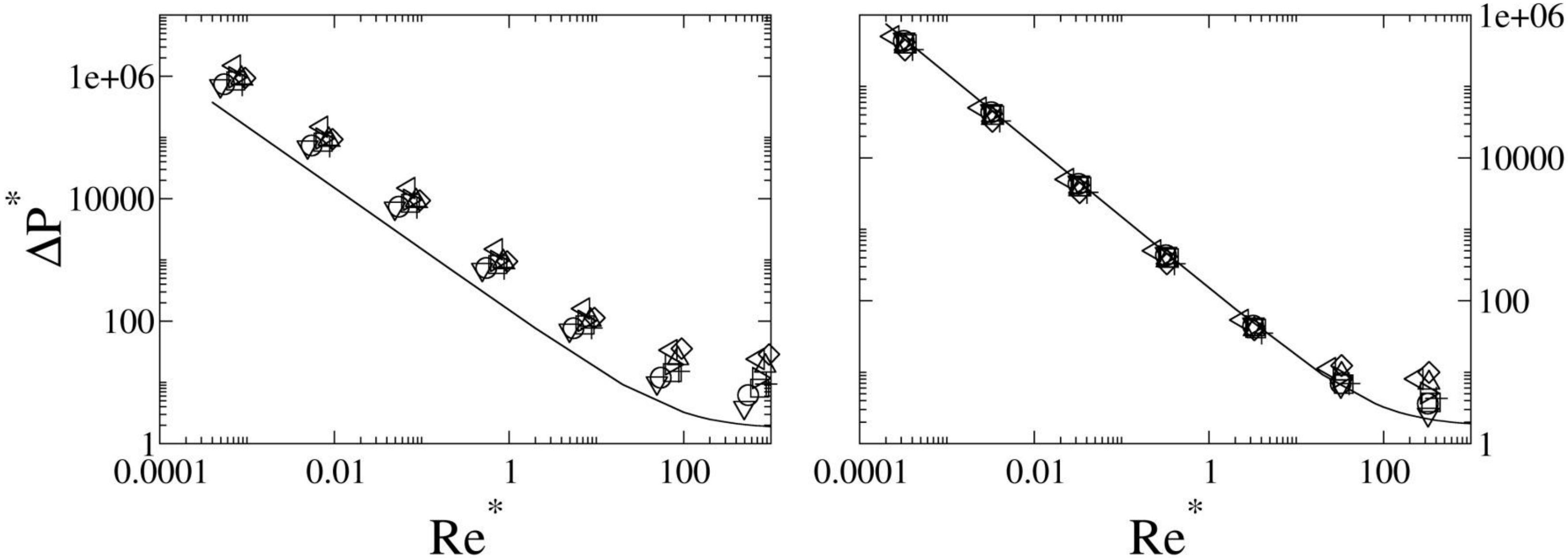
- 8 realistic geometries

- 4 simplified geometries



RESULTS: FLUID FLOW

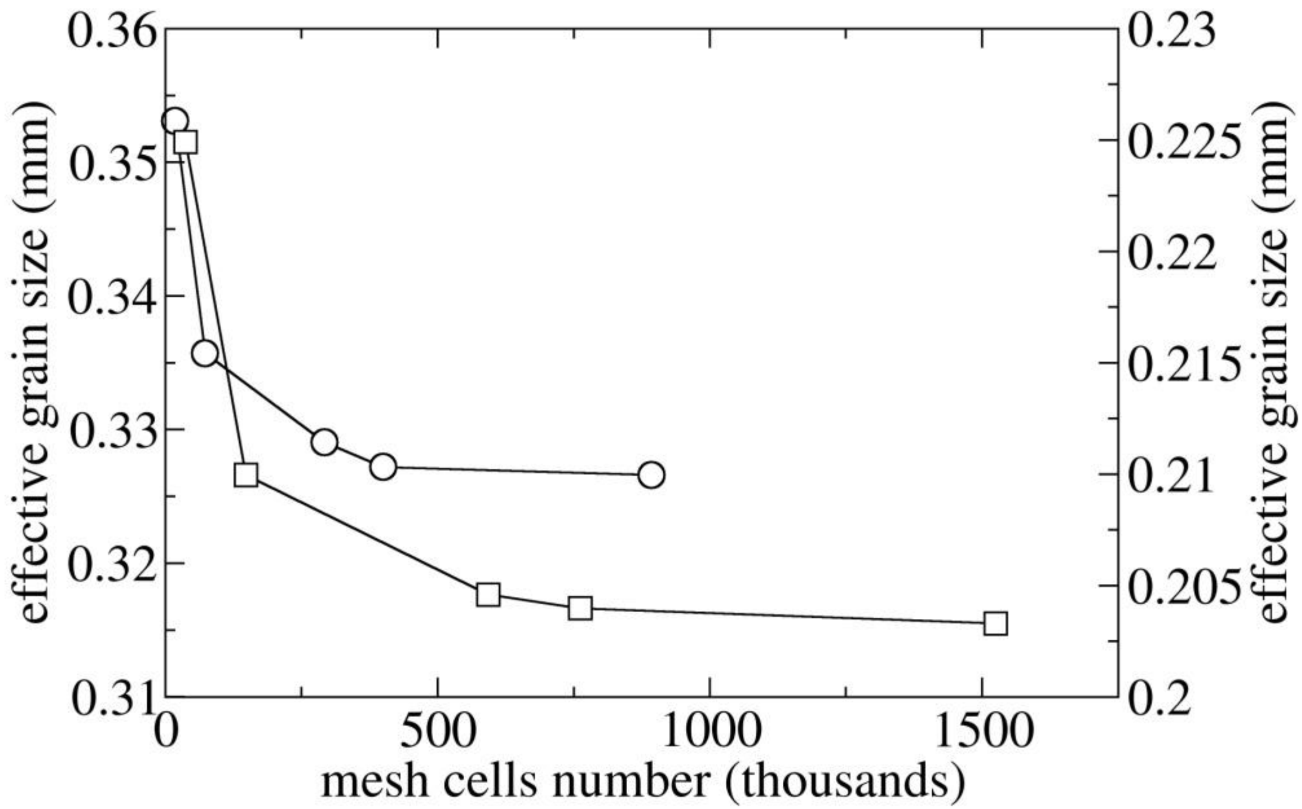
COMPARISON WITH ERGUN'S LAW



- Results show good agreement with Ergun's law
- Fitting on Ergun's law to obtain an <u>effective</u> grain diameter, D_g^*

Results: fluid flow

Grid Independence Verification



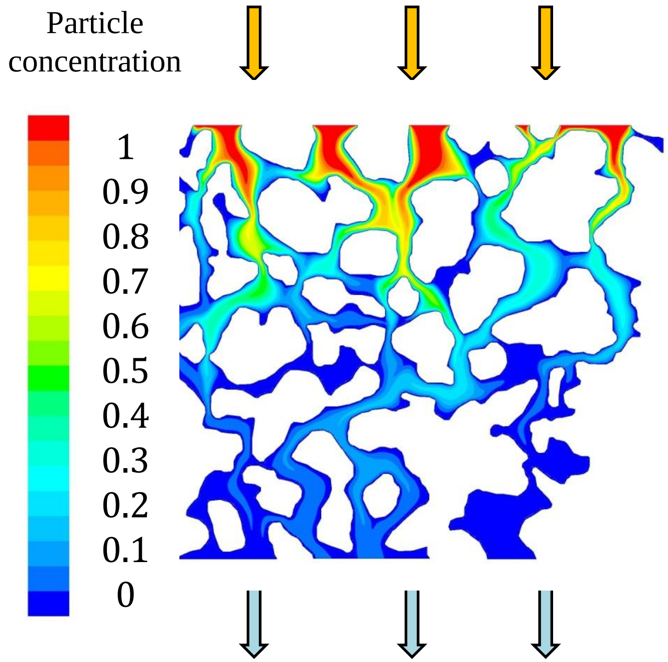
- Need for a single parameter summarizing fluid flow results
- Grid independence assessed with changes in D_g^*

METHODOLOGY: OPERATING CONDITIONS

PARTICLES MODELING

- Particles are transported by convective and diffusive phenomena
- C = 1 at inlet
- C = 0 on grain surface
  - Assumed "perfect sink" condition
- Particle diameter

  d_p = 1, 10, 100, 200, 500, 625, 750, 875, 1000 nm

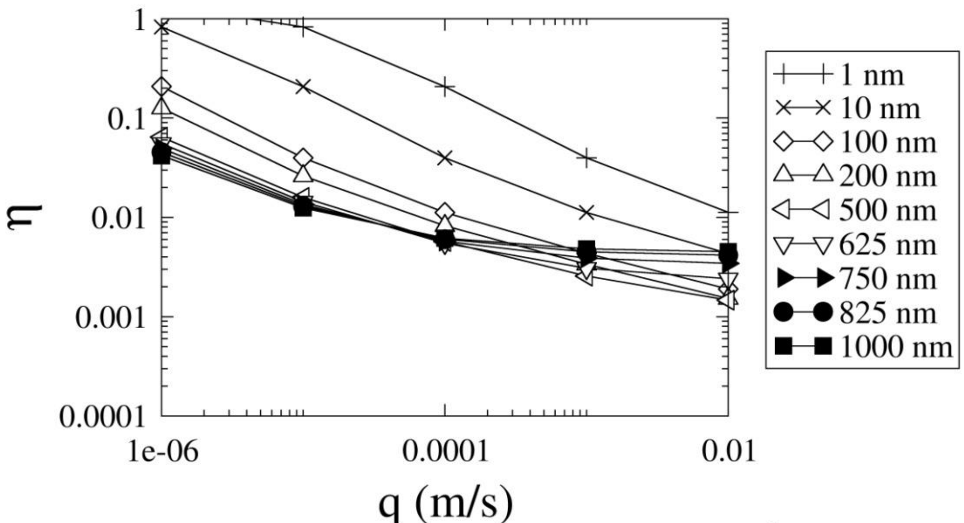


Collector deposition efficiency, η
calculated with packed bed performance equation

$$\frac{dC}{dx} = -\frac{3}{2}\frac{1-\varepsilon}{\varepsilon D_g}\eta C$$

RESULTS: PARTICLE DEPOSITION

DEPOSITION EFFICIENCY: OVERVIEW

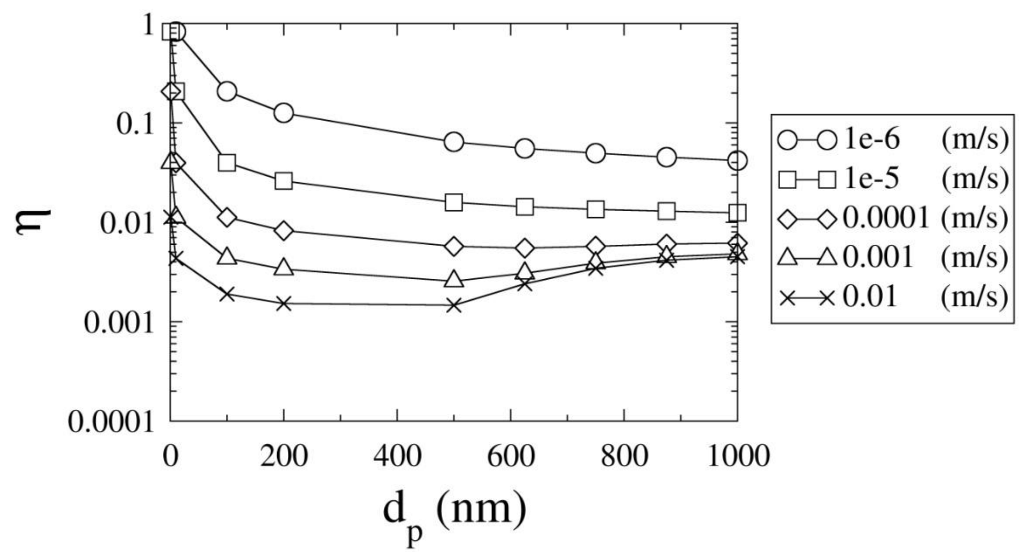


Efficiency η decreases for higher superficial velocities *q*

(low residency times)

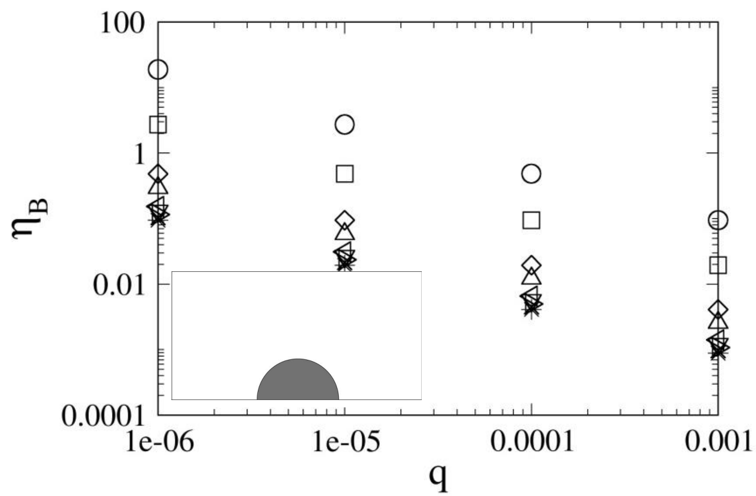
Efficiency η decreases for higher particle diameter

(low diffusivity) until a certain *dp* value, then increases for the steric interception effect.



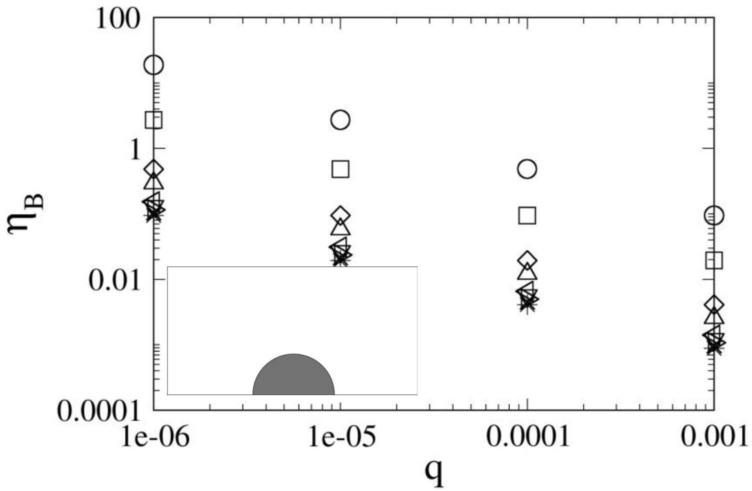
RESULTS: PARTICLE DEPOSITION

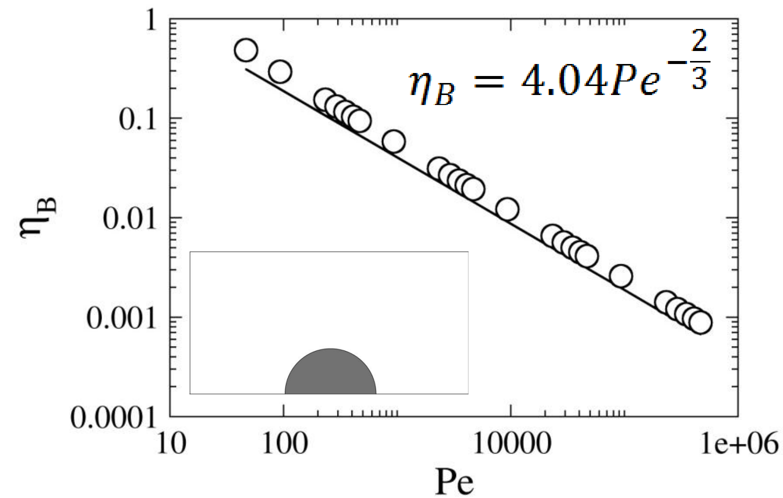
DEPOSITION EFFICIENCY: BROWNIAN DIFFUSION



RESULTS: PARTICLE DEPOSITION

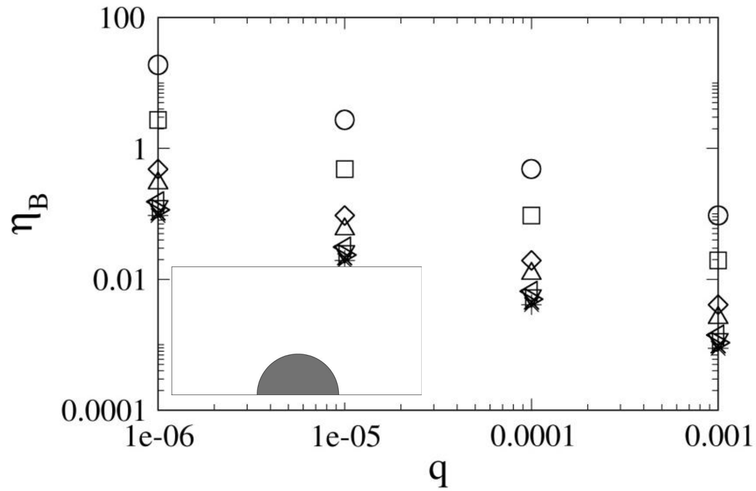
DEPOSITION EFFICIENCY: BROWNIAN DIFFUSION

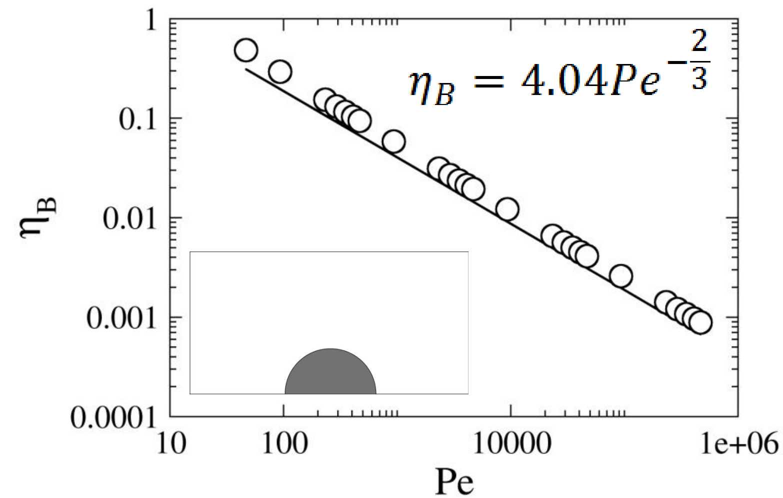


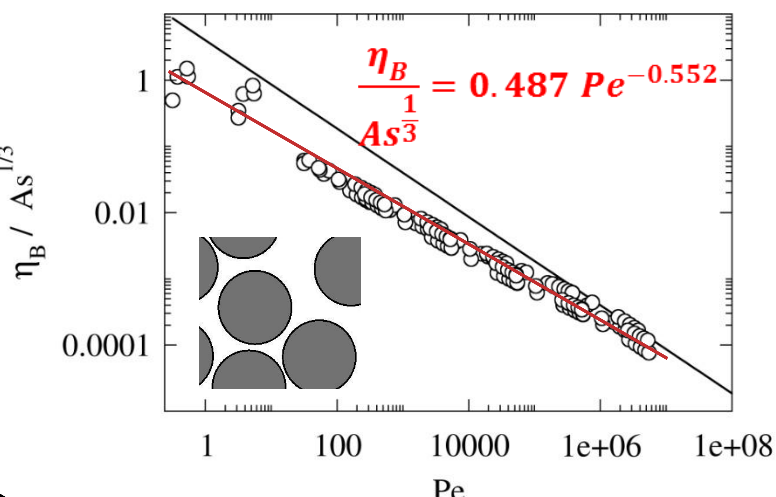


Results: particle deposition

Deposition Efficiency: Brownian Diffusion

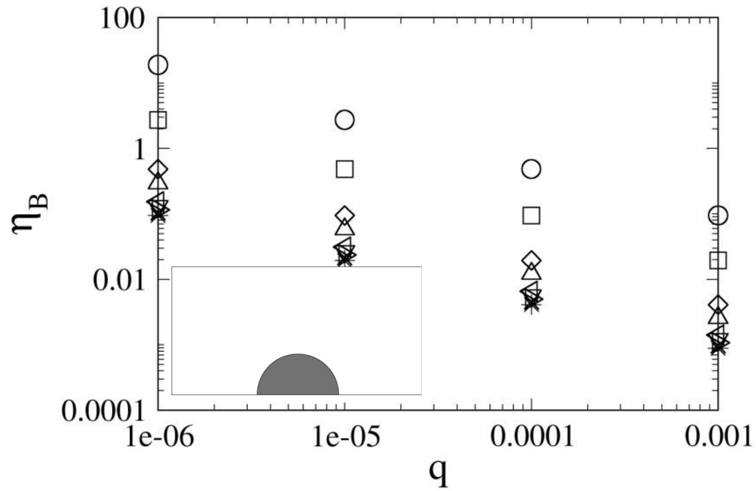


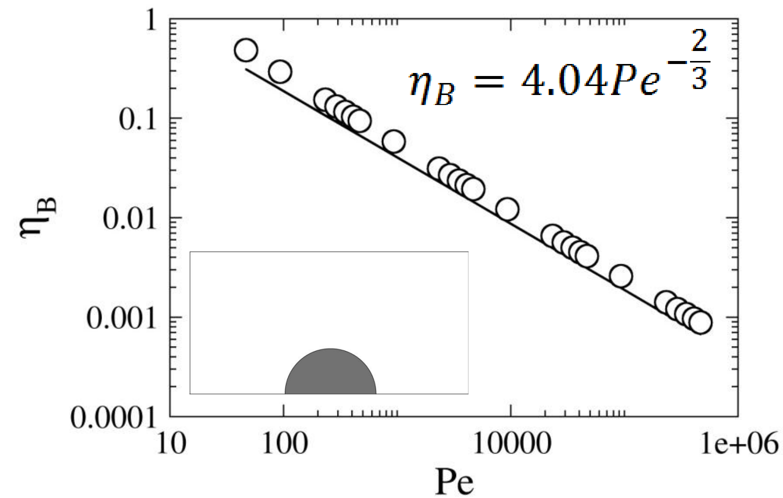


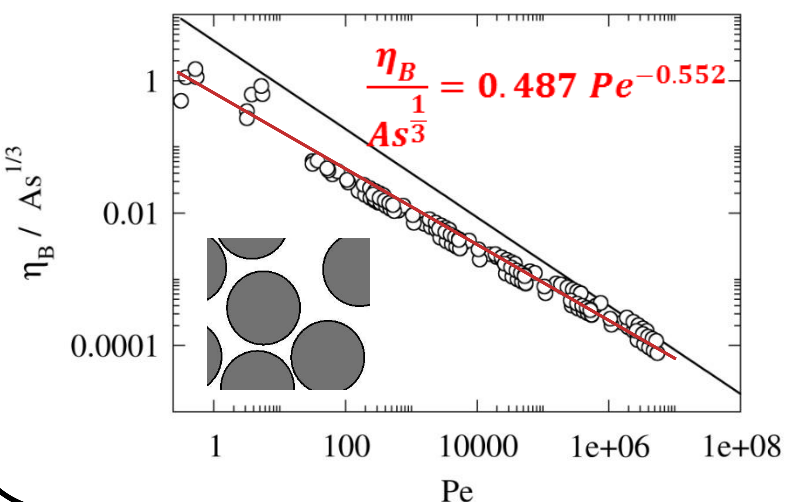


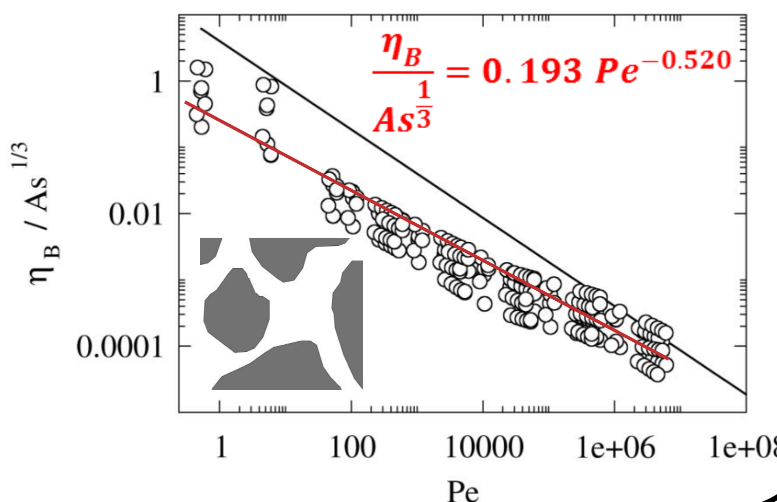
RESULTS: PARTICLE DEPOSITION

DEPOSITION EFFICIENCY: BROWNIAN DIFFUSION



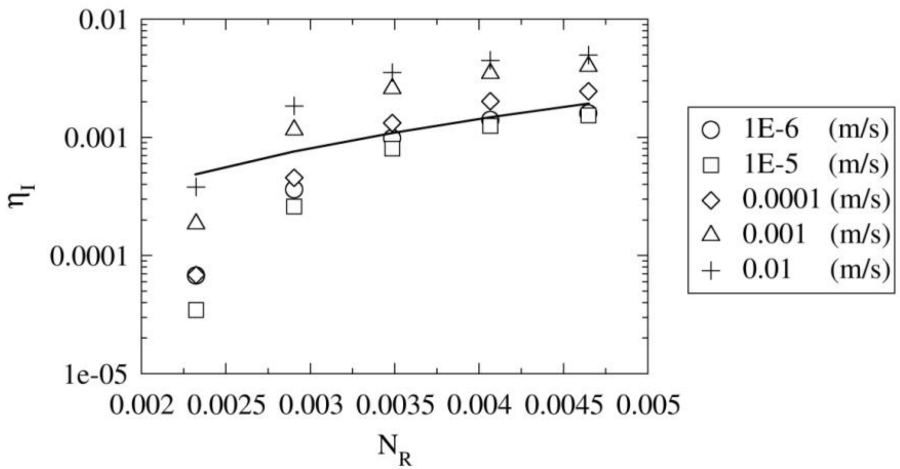






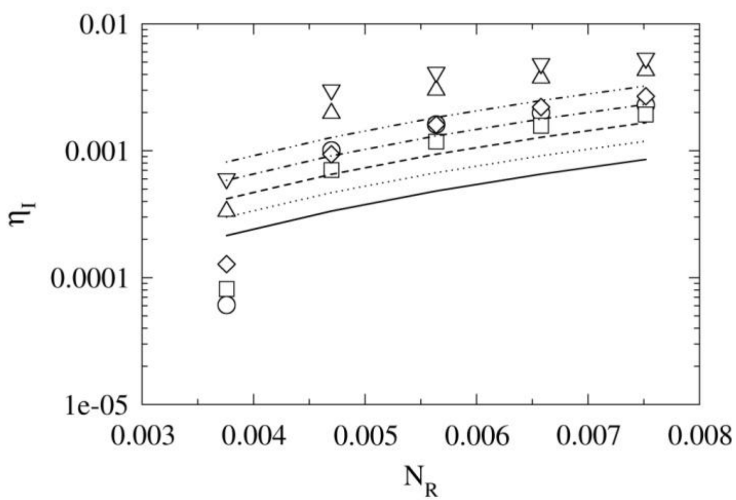
RESULTS: PARTICLE DEPOSITION

DEPOSITION EFFICIENCY: INTERCEPTION



Theoretical law:

$$\eta_I = \frac{3}{2} As \, N_R^2$$

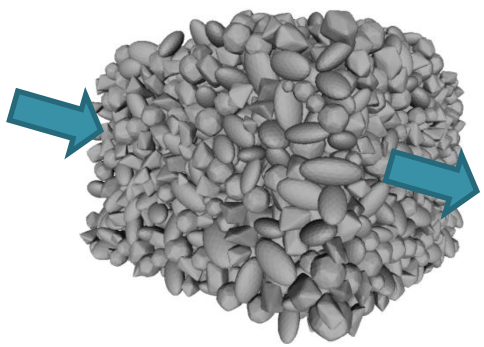


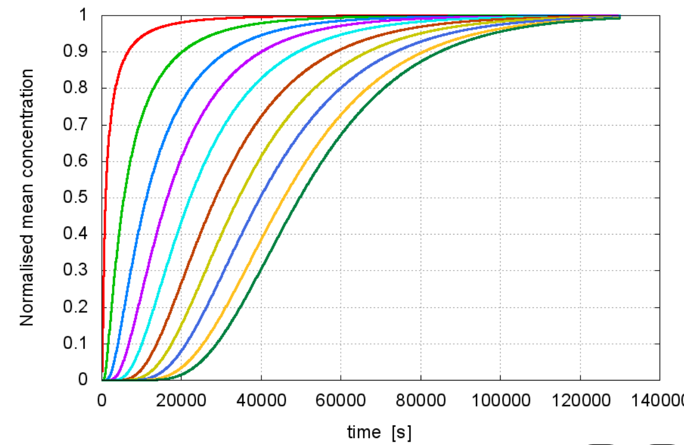
- Results appear in line with theoretical predictions but are strongly dispersed, with great variations at different q
- A dependency of η on q can be proposed

$$\eta_I = 3.377 \, As \, N_R^2 \, q^{0.145}$$

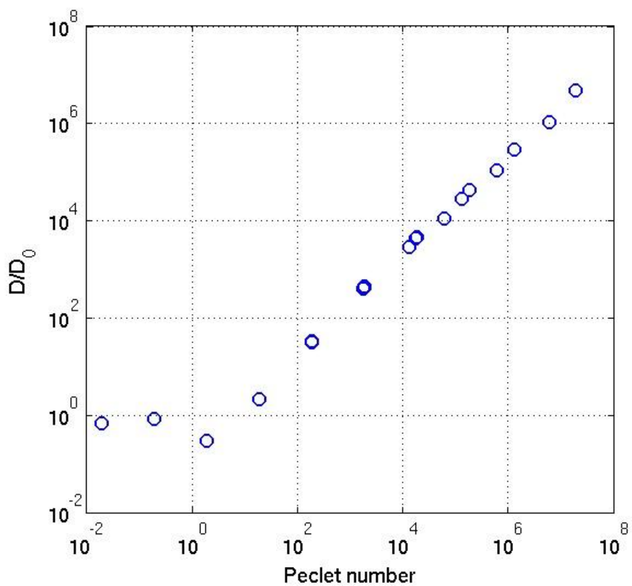
Conclusions and Future work

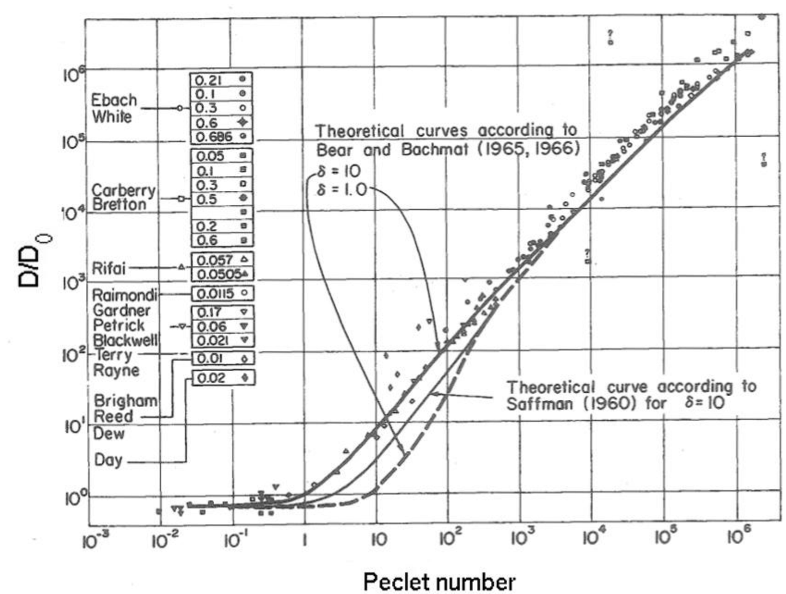
Fully 3D Particle transport simulations





Breakthrough curves fitting → Hydrodynamic dispersion $\mathcal{D}/\mathcal{D}_0$ results





Conclusions and Future work

Acknowledgements

- AQUAREHAB (FP7, Grant Agreement no. 226565)
- PRIN Project 2008:

  "Disaggregazione, stabilizzazione e trasporto di ferro zerovalente nanoscopico"

Thanks for your attention!

Any questions?